

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.65

Global applicability domain: Outside

Local applicability domain index: 1.98e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Malaoxon</div> <div>Measured: 1.12</div> <div>Predicted: 1.49</div>	<div>Image not found</div> <div>Tris(2-hydroxyethyl) isocyanurate</div> <div>Measured: 1.58</div> <div>Predicted: 1.61</div>	<div>Image not found</div> <div>Tris(2-butoxyethyl) phosphate</div> <div>Measured: 5.75</div> <div>Predicted: 6.32</div>
<div>Image not found</div> <div>N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine</div> <div>Measured: 3.47</div> <div>Predicted: 4.50</div>	<div>Image not found</div> <div>Malathion</div> <div>Measured: 33.1</div> <div>Predicted: 21.9</div>	